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13. ABSTRACT (Maximum 200 words)

This has been an exceptionally productive 3 years. We have several papers published in the best journals in the area, several are in review, and a new and promising avenue of research has been opened by our first paper of our renewal project. This new research began under the current project. Indeed, there have been two international workshops, one in Denmark and one in Portugal, inspired by our work, and we were invited to edit a special issue of Optimization in Engineering with Professor Luis Vicente of Coimbra, who received his PhD with Dennis at Rice.

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Optimization Tools for Engineering Design
Using Surrogate Functions

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February 2004

Status of Effort:

This has been an exceptionally productive 3 years. We have several papers published in the best journals in the area, several are in review, and a new and promising avenue of research has been opened by our first paper of our renewal project. This new research began under the current project. Indeed, there have been two international workshops, one in Denmark and one in Portugal, inspired by our work, and we were invited to edit a special issue of *Optimization in Engineering* with Professor Luis Vicente of Coimbra, who received his PhD with Dennis at Rice.

Gilles Couture has completed design cycle 5 of NOMAD-C++. The code and documentation are available at http://www.gerad.ca/NOMAD/ . NOMAD can solve general nonlinearly constrained optimization problems with continuous variables with either GPS or MADS. It has a graphical user interface and a database to avoid function evaluations redundancy. We were greatly aided in this effort by Dr. Steve Thomas. Thomas is now manager of the High Performance Computing Group at SANDIA Livermore Laboratory. He continues to provide valuable software engineering guidance, although now his effort is supported by CSRI, the Computer Science Research Institute of SANDIA Labs.

Presently, NOMAD is being used in an ExxonMobil internal software package to determine the constituents of each tanker of oil for product planning purposes. Previous approaches could sometimes hold up the process for over a day, while NOMAD has never needed more than 15 minutes to solve an instance of the problem. ExxonMobil is having preliminary success with NOMAD on a subproblem of the well bore trajectory problem. This is a very interesting application for our further algorithm development.

The DAKOTA project at SANDIA National Labs has approached us about adding NOMAD to its software framework to handle derivative free optimization. They will support this development.

We have recently made an important breakthrough in both the theory and

the practice of derivative-free methods. Our new research eliminates the main limitation of the Generalized Pattern Search (GPS) class of algorithms, which formed the algorithmic infrastructure for our past work. Our new work addressed the issue that the GPS algorithm class relies heavily on a fixed finite set of directions, and that the convergence results are heavily tied to these directions. We found a way to lift this restriction, and now we allow the algorithm to explore in a set of directions which is dense in the entire space. We call this the Mesh Adaptive Direct Search (MADS) class of algorithm, and it generalizes GPS. We observed significant improvements on some interesting problems.

Lt Col. Mark Abramson, a PhD student produced jointly by Audet and Dennis during the period being reported upon, is working with us to draft a graduate level engineering and applied mathematics textbook based on our research. In addition, Lt Col Abramson is showing himself to be a valuable and active independent researcher. He is our best transition to the USAF. His dissertation is available from www.caam.rice.edu as TR02-11, and several subsequent papers can be found there as well.

Two students started the courses for their Ph.D. in Montréal under the supervision of Audet, and will work on extensions of MADS. Sébastien Le Digabel's B-exams were held in January 2004, and Walid Zghal will take these exams in July 2004. John Dennis is on the PhD committee of Parvez Moin's Stanford graduate student Alison Marsden, whose dissertation deals with applying the surrogate management framework to obtain quiet airfoil designs.

Accomplishments/New Findings:

Especially noteworthy accomplishments are:

- Several papers have appeared or been accepted by top peer reviewed

journals. Our papers combine theoretical results, analysis of the limitations of GPS and numerical results on some real engineering problems.

- The new MADS framework will replace our GPS framework. MADS is much more flexible, and allows us to show the convergence results that we always wished for in GPS, but knew did not hold. This opens the door for updating all our previous papers into this new framework. This will be done in the book.

- Cycle 5 release of NOMAD C++ software. NOMAD can now solve general nonlinearly constrained optimization problems using the filter method, and treat bound constraints by the barrier approach, and by making sure that the directions conform to the boundary of the box. User-defined surrogates can now be used together with NOMAD. A mechanical engineering masters student tested this feature using his own surrogate model. Latin hypercube random searches can now be performed. MADS algorithm are coded and tested on several test problems.

  Cycle 5 is used at United Technologies Research Center and at Exxon-Mobil Upstream Research Company. We are negotiating with SANDIA National Labs to include NOMAD in their DAKOTA framework for engineering design.

- GPS and MADS were used to evaluate kinetic parameters from light-off curves for a catalytic reactor (such as an automobile catalytic converter). The "honeycomb " design contains hundreds of cells of the order of 1 mm and may have a variety of cross sectional shapes and different substrate materials. The four-variable problem that we looked at is a simplification of the real one. GPS algorithm found better solutions faster than a gradient-based method. MADS was even faster than GPS.

- In order to compare several algorithms designed to handle black box functions, Professor C. T. Kelley made public a series of non-linear well location optimization problems that require the use of a flow solver to evaluate the objective function. Kelley will publish the numerical results for 6-8 different software packages, including our NOMAD. Our preliminary results show that NOMAD often improved the initial so-

lution at a rate faster than the other methods, and often produced the best overall solution.

Personnel Supported:

Faculty: Professor John Dennis and Professor Charles Audet
Research Staff: Gilles Couture and Dr. Steve Thomas

Publications:

Published:

- Sethi, S., M.R. Wiesner, and J. E. Dennis, Optimization of Hollow-Fiber Design and Low-Pressure Membrane System Operation, *Journal of Environmental Engineering* 127(6), pp. 485-492, 2001.

- Alarie, S., C. Audet, B. Jaumard and G. Savard, Concavity Cuts for Disjoint Bilinear Programming, *Mathematical Programming* 90(2), pp 373–398, 2001.

- Audet, C., P. Hansen, B. Jaumard and G. Savard, Enumeration of All Extreme Equilibria of Bimatrix Games, *SIAM Journal on Scientific Computing*, 23(1), pp 323–338, 2001.

- Kokkolaras, M., C. Audet, and J. E. Dennis, Jr, "Mixed Variable Optimization of the Number and Composition of Heat Intercepts in a Thermal Insulation System". *Optimization and Engineering*, 2(1), pp 5–29, 2001.

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- Audet, C., P. Hansen, F. Messine, and J. Xiong, "The Largest Small Octagon", *Journal of Combinatorial Theory, Series A*, 98(1), pp 46–59, 2002.

- Dennis, J.E. Jr. and Zhijun Wu "Parallel Continuous Optimization," in *The Sourcebook of Parallel Computing*, ed by Dongarra, Foster, Fox, Gropp, Kennedy, Torczon, White, pp 612-634, 2002

- Audet C. and Dennis J.E.Jr, Analysis of Generalized Pattern Searches, *SIAM Journal on Optimization*, Vol.13 No.3, 889-903, 2003.

Accepted for Publication:

- Audet C. and Dennis J.E.Jr (2000), A Pattern Search Filter Method for Nonlinear Programming without Derivatives, TR00-09 Department of Computational and Applied Mathematics, Rice University, Houston, (to appear in *SIAM Journal on Optimization*).

- Abramson M.A., Audet C. and Dennis J.E.Jr (2002), Generalized Pattern Searches with Derivative Information, *Les Cahiers du GERAD G-2002-28*, Montréal, (to appear in *Mathematical Programming, series B*).

- Audet C. (2002), Convergence Results for Pattern Search Algorithms are Tight, *Les Cahiers du GERAD G-2002-56*, Montréal. To appear in *Optimization and Engineering*.

- Audet C., Carrizosa E., Hansen P.(2000), An Exact Method for Fractional Goal Programming, *Les Cahiers du GERAD G-2000-64*, Montréal. To appear in *Journal of Global Optimization*.

- Audet C., Hansen P. and Le Digabel S. (2003), Exact solution of three nonconvex quadratic programming problems, Les Cahiers du GERAD G-2000-23, Montréal. To appear in the book series *Nonconvex Optimization and its applications*, Kluwer Academic Publishers.

- Audet C., Brimberg J., Hansen P., Le Digabel S. and Mladenovic N. (2000), Pooling Problem: Alternate Formulations and Solution Methods, *Les Cahiers du GERAD G-2000-23*, Montréal. To appear in *Management Science*.

- Dennis, J. E., C. Price and I. Coope, Direct Search Methods for Non-linearly Constrained Optimization Using Filters and Frames, to appear in *Optimization and Engineering*.

- Hayes R.E., Bertrand F.H., Audet C., Kolaczkowski S.T.(2002), Catalytic combustion kinetics: Using a direct search algorithm to evaluate kinetic parameters from light-off curves, *Les Cahiers du GERAD G-2002-20*, Montréal. To appear in *The Canadian Journal of Chemical Engineering*.

Submitted for Publication:

- Audet C. and Dennis J.E.Jr , Mesh Adaptive Direct Search Algorithms for constrained optimization Les Cahiers du GERAD, (submitted to *SIAM Journal on Optimization*), 2003.

- Audet, C., P. Hansen, F. Messine, S. Perron "The Minimum Diameter Octagon with Unit-Length Sides: Vincze's Wife's Octagon is Suboptimal", Les Cahiers du GERAD G-2003-59 (submitted to *Journal of Combinatorial Theory, Series A*), 2003.

- Audet, C., S. Belhaza, P. Hansen (2003) "Enumeration of All Extreme Equilibria in Game Theory: Bimatrix and Polymatrix Games", Les Cahiers du GERAD G-2003-63 (submitted to *Journal of Optimization Theory and Applications*), 2003.

- Dennis, J. E., Olga A. Brezhneva, Pattern Search Methods for Linearly Constrained Minimization in the Presence of Degeneracy, submitted for publication, available as IMA Preprint series, # 1934, and Rice CAAM-TR03-09, August 2003.

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- Marsden, Alison, Meng Wang, J. E. Dennis, and Parviz Moin) Optimal aeroacoustic shape design using the surrogate management framework, submitted for publication.

Interactions and Transitions:

Public Presentations:

J. E. Dennis

- "Optimization using Surrogates for Engineering Design". Los Alamos National Labs. October 15, 2001

- "A Rigorous Framework for Surrogate Optimization". Optimization Planning Day, United Technologies Research Center, West Hartford, Connecticut, October17,2001

- "Mixed Variable Programming". United Technologies Research Center, West Hartford, Connecticut, October 22,2001

- "Optimization using Surrogates for Engineering Design". Undergraduate Mathematics Club, Trinity University, San Antonio, Texas, November 8, 2001.

- "Working with Industry - My Life as an Evangelist". Computer and Information Technology Institute, Rice University, December 7, 2001.

- "Progress on the Surrogate Management Framework", ExxonMobil Upstream Research Company, December 12, 2001

- "Optimization using Surrogates for Engineering Design". Computational and Applied Mathematics, Rice University, January 14, 2002.

- "Optimization using Surrogates for Engineering Design". 10 hour shortcourse at University of Cantebury, Christchurch, New Zealand, February 15-March 29, 2002

- "Optimization using Surrogates for Engineering Design". 10 hour short-course at University of Coimbra, Coimbra, Portugal, May 6-10, 2002

- "Analysis of Generalized Pattern Search Algorithms". Second international workshop on surrogate modelling for engineering optimization; Coimbra, Portugal; May 16, 2002.

- "Analysis of Generalized Pattern Search Algorithms". SIAM Meeting on Optimization; Toronto, Canada, May 21, 2002.

- "A Filter Approach to Derivative-Free Constrained Optimization". Keynote Address at Argentine-Brazilian Workshop on Continuous Optimization, Institute for Pure and Applied Mathematics, Rio de Janeiro, Brazil, July 15, 2002.

- "Optimization using Surrogates for Engineering Design". Plenary address at 30th Anniversary Workshop for the NASA Institute for Computer Applications in Science and Engineering. Hampton, Virginia, July 25, 2002.

- "Optimization using Surrogates for Engineering Design". State-of-the-field address at Los Alamos Computer Science Institute Annual Meeting, Sante Fe, October 15, 2002.

- "Optimization Tech Transfer is a Two-Way Street". ExxonMobil Upstream Research, November 5, 2002.

- "Infrastructure for Surrogate Optimization". 3-hour shortcourse, Exxon-Mobil Upstream Research, November 6, 2002.

- "Optimization Using Surrogates for Engineering Design - A Use for Uncertainty Quantification". Los Alamos Predictability Meeting, Sante Fe, December 16, 2002.

- "Industrial Strength Optimization". A 6 hour short course at the Institute for Mathematics and Its Applications, University of Minnesota, January 2003

- "Working with Industry - My Life as an Evangelist". Graduate Student Colloquium, Institute for Mathematics and Its Applications, University of Minnesota, February 2003

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- "Early Career Issues for Mathematicians". Graduate Student Colloquium, Institute for Mathematics and Its Applications, University of Minnesota, February 2003

- "Optimization Technology Transfer is a Two-Way Street", Optimization Colloquium, Institute for Mathematics and Its Applications, University of Minnesota, February 2003

- "Generalized Pattern Search Algorithms for Mixed Variable Programming". Numerical Analysis Seminar, Department of Mathematics, University of Minnesota, February 2003

- "Two lectures on some mathematics of engineering design requiring at most linear algebra and vector calculus and at least an open mind", Junior Colloquium, Department of Mathematics, University of Minnesota, February 2003

- "Optimization using Surrogates for Engineering Design". Department of Mathematics, University of Minnesota, March 15, 2003

- "Working with Industry - My Life as an Evangelist". Graduate Student Brown Bag Colloquium, Iowa State University. March 22, 2003

- "Optimization using Surrogates for Engineering Design". Iowa State University. March 22, 2003

- "Optimization using Surrogates for Engineering Design". AFOSR PI meeting, Estes Park, CO. May 27, 2003

- "Derivative assisted Pattern Search Methods". SIAM Annual Meeting, Montreal, CA. June 20, 2003

- "Industrial Strength Optimization". A 4 hour short course given with Lt Col Mark Abramson at AFIT, August 7, 2003

- "Optimization for Engineering Design using Surrogates". Homer Walker Birthday Symposium, WPI, Worchester, MA. September 20, 2003

- "Mesh Adaptive Direct Search Algorithms". LACSI Annual Meeting, Sante Fe, NM, October 27, 2003

- "Optimization using Surrogates for Engineering Design". Fluids Colloquium, Mechanical Engineering Department, Stanford University, November 11, 2003.

- "Optimization using Surrogates for Engineering Design". Los Alamos National Lab, November 18, 2003.

- "Mesh Adaptive Direct Search Algorithms". Los Alamos National Lab, November 18, 2003.

- "Optimization using Surrogates for Engineering Design". ExxonMobil Upstream Research Co., December 1, 2003.

- "Mesh Adaptive Direct Search Algorithms". CAAM Department, Rice University, December 2, 2003.

- "Mesh Adaptive Direct Search Algorithms". Mathematics Department, Emory University, December 5, 2003.

Charles Audet

- "First Order Optimality Conditions Tied to Local Differentiability". *International Symposium on Mathematical Programming*, Denmark, Aug 2003.

- "First Order Optimality Conditions Tied to Local Differentiability". *SIAM annual meeting*, Montréal, Canada, June 2003.

- "A Cuts Algorithm for the Linear Bilevel Programming Problem". *Optimization Days*, Montréal, Canada, May 2003.

- "The Pooling Problem: Alternate Formulations and Solution Methods". *Optimization Days*, Montréal, Canada, May 2003.

- "First Order Optimality Conditions Tied to Local Differentiability". *Optimization Days*, Montréal, Canada, May 2003.

- "Industrial strength optimization". *IMA 6 hours short course : Optimization*, University of Minnesota, Jan 2003.

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- "Generalized Pattern Searches with Complete or Incomplete Derivative Information". *Optimization Days*, Montréal, Canada, May 2002.

- "The largest small octagon". *Optimization Days*, Montréal, Canada, May 2002.

- "Generalized Pattern Searches with Complete or Incomplete Derivative Information". *Second international workshop on surrogate modelling for engineering optimization*, Coimbra, Portugal; May 2002.

- "Generalized Pattern Searches with Complete or Incomplete Derivative Information". *SIAM Meeting on Optimization*, Toronto, Canada, May 2002.

Editorial positions:

J. E. Dennis

2001–	Editorial Board, *SIAM Journal on Optimization*
1992–	Advisory Editor, *Mathematics of Operations Research*
1999–2003	Editor-in-Chief and Founder, *MPS/SIAM Book Series on Optimization*
2003	Invited Editor for *Optimization and Engineering* (special issue on Surrogate Optimization)

Charles Audet

2003 Invited Editor for *Optimization and Engineering* (special issue on Surrogate Optimization)

2003 Editor for *Essays and Surveys in Global Optimization* (Kluwer) commemorating the 25th anniversary of the GERAD research center.

Consultative and Advisory Functions:

J. E. Dennis

- One day per week at Boeing Phantom Works Mathematics and Engineering Analysis Group working on Design Explorer Project and Systems of Systems optimization.

- Summer Quarter at University of Canterbury, New Zealand as an Erskine Fellow. Gave a 10 hour shortcourse on this project.

- Spring Term as Professor at the University of Coimbra. Gave a 10 hour shortcourse on this project.

- Advisory Committee for Worcester Polytechnic Institute.

- ExxonMobil Upstream Research Company

- United Technologies Research Center

- SANDIA National Labs

- Lawrence Berkeley Laboratory Nanotechnology workshop

- Named to PhD committee for Stanford University Mechanical Engineering doctoral candidate Alison Marsden

Transitions:

Projects in the Exploratory Stage

- **Well casing** All four of the personnel who received support from this grant spent some time at ExxonMobil Upstream Research Company talking about various collaborations. One problem presently being discussed is an interesting mixed integer problem, which is described

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briefly as follows. As a well is being drilled, it is important to insert sleeves of well casing to keep the sides of the hole from collapsing into the well. The first sleeve is the largest in diameter, the second is inserted inside the first and lowered into place, and this concentric sleeving continues until the drilling is completed and the wall of the well is completely reinforced by concentric sleeves of decreasing diameter. The problem is to determine the number of sleeves, a categorical variable, and the length and diameter of each sleeve for a well of given depth. Of course, there are various structural constraints, and cost is the objective to be minimized. We should be able to deal with this problem with little difficulty, but the delay is due to a need to obtain internal funding for ExxonMobil personnel to gather all the necessary simulation routines. The status of this project is that NOMAD has been successfully used by ExxonMobil to solve the problem for a single section.

Contact: Dr. Amr ElBakry (713)431-7137.

- **Boeing - UTRC Collaboration** In early September, Dennis will participate in a one day exploratory meeting to discuss a collaboration between Mathematics and Engineering Analysis at Boeing Phantom Works, the Mathematics group at United Technology Research Center (UTRC), and the High Performance Computing group at Lawrence Berkely Labs. The goals of this collaboration will be set later, but one of the major objectives of this research is to influence the way design problems are solved in industry. However, it seems clear that a parallel version of our algorithms will be one of the goals since this is the main interest of our LBL collaborators.

Dr. Evin Cramer (206)232-9577

- **Nozzle Design** Our group continues working with a group in Boeing Commercial Airplane Group (BCAG) to reduce the cycle time for designing nozzles. A nozzle is the inside part of the engine housing, and its design is affected by the design of the more "upstream" components. This means that many of the design changes involving other airplane components force a redesign of the nozzle as well.

A nozzle design is specified by 100 parameters, 90 of which are fixed by other considerations. The system is governed by a 2D Navier Stokes

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coupled with NASTRAN, a commercial structures code. It takes about 3 hours on an SGI Challenge to get one function value. The current length of a design cycle is two weeks. We expect to reduce that to approximately one day.

This project has been delayed by the higher internal Boeing priority of the planform project.

Contact: Dr. Evin Cramer (206)232-9577 or
          Dr. Greg Shubin (425)865-3516.

Ongoing Projects

- **Model Management Framework Software** Boeing has the latest NOMAD-C++ release as well as the NOMADm MatLab software. When internal funding permits, this will likely become the basis for reimplementation of their Design Explorer Software. This implementation replaces the C++ box constrained prototype delivered previously. The framework can be used to develop model management algorithms specialized for a user's applications and capabilities. The Boeing version of our work, Design Explorer, is presently being commercialized by Phoenix Integration.

Contact: Dr. Evin Cramer (206)232-9577 or
          Dr. Greg Shubin (425)865-3516.

- **Planform Design** Our algorithms were used in a production environment by Boeing in planform design for the near sonic cruiser. This was done by the BCAG group that does planform design. The decision was made not to build this airplane because of economic conditions in the airline industry. Now, Design Explorer is being used on the proposed Dreamliner 7e7. Boeing continues to achieve better planforms with greatly reduced cycle time.

The planform is the shape of the wing as viewed from above. It is a tricky design problem that involves a couple of dozen variables and some interesting constraints. For example, the fuel is outboard on the wings, and the wings must be swept back for performance. One constraint is that the plane must not fall over backwards when the

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tanks are filled while the plane is on the ground. This problem involves multiple objectives and discrete variables, but the first test problem run by Boeing used cost/passenger mile as objective and assumed values for the discrete variables, like where the wings are placed on the body.

The following text on the recent test was approved by Boeing for release:

Recent Product Development activities at Boeing have underscored the need to decrease the time to market and cost of products. To accomplish this, Boeing has been examining all of its processes in development and production.

One process in particular that occurs early in the design is the determination of a wing planform, which must be chosen to meet mission while decreasing operating economics and respecting design constraints. Boeing is exploring whether this highly multi-disciplinary problem yields itself to integrated analysis and optimization techniques, with the hope of decreasing the cycle time of finding a preferred result by an order of magnitude.

This exploration provided the Design Explorer Team, of which Rice is a member, with an opportunity to apply our design optimization tools. It has also been useful from the standpoint of exercising the various discipline analysis tools. Starting from baselines developed through the standard process and using a significant subset of the tools, we have been able to demonstrate actual integration of the analyses from the different disciplines and the speed advantages that we were looking for. The solutions found do, within the level of accuracy of the included tools, meet all constraints while showing economic benefit relative to our analyses of the initial baselines.

The approach to this problem used response surface (surrogate) modeling to speed up the optimization, as opposed to continuously resampling the analysis tools. Of additional note is that incorporation of Model Management Framework elements into the optimization scheme allowed resolution of the selected optimum to search variables of second order importance. Such resolution is particularly difficult to obtain when using response surface modeling.

Contact: Dr. Evin Cramer (206)232-9577 or
Dr. Greg Shubin (425)865-3516.

- **Boeing Parts Nesting System** PDS continues to be used in the Boeing Parts Nesting System 2NA for just-in-time manufacturing of aircraft parts. This code runs over 100,000 times per day.

Inventions, or Patent Disclosures:

None.

Honors/Awards:

J. E. Dennis

- Very Important Visitor at Institute for Mathematics and its Applications at the University of Minnesota Winter 2003

- Ordway Distinguished Lecturer in the Mathematics Department at the University of Minnesota Winter 2003

- Chair of the organizing committee for the SIAM 2004 Annual Meeting to be held in Portland, OR

- Named a HighlyCited Computer Scientist by ISI.

- Dedicatee of special issue of the *SIAM Journal on Optimization* (Volume 9, Number 4) `<http://epubs.siam.org/sam-bin/dbq/toc/SIOPT/9/4>`.

- Chair(President) of the Mathematical Programming Society

- Founder and Editor-in-Chief of MPS/SIAM Book Series on Optimization

- Advisory Editor, *Mathematics of Operations Research*, (1992—).

- Founding Editor-In-Chief of *SIAM Journal on Optimization.*

- Served on and chaired numerous panels and visiting committees.

- Served two terms on the SIAM Council.

- Fulbright Lecturer to Argentina.

- Twice an Erskine Fellow at the University of Canterbury, Christchurch, NZ, 2000 and 2002, and the third fellowship will take place during February and March 2004.

Charles Audet

- Promotion to the tenured rank of *Assistant Professor* after only three years of experience.

- Charles Audet has received two Canadian young researcher awards: Strategic NATEQ professor-researcher, and a CFI subvention with 7 other professors at Ecole Polytechnique.